PhD SCHOLARSHIP APPLICATION FORM 2016

ORGANISATION Business Division Business Area	**TECNALIA RESEARCH & INNOVATION** SUSTAINABLE CONSTRUCTION Innovative & Sustainable Materials:
Scholarship location Province/Building	BIZKAIA, Parque Tecnológico de Bizkaia, Edificio 700-Derio
Tutor	Dr Jorge Sánchez Dolado

SCHOLARSHIP DESCRIPTION

Title: Ultra-reactive Cement and Pozzolan Design through Multi-Scale Model Simulation

Brief Description of Scholarship:

One of the objectives most desired by the cement industry is to increase cement and pozzolan hydration rate. This will enable: reduced construction times and costs; cutting down on the use of accelerators; minimise the use of natural resources using pozzolans as supplementary materials; and use belite cements to reduce CO_2 emissions. Today, and despite the large number of empirical studies, those targets have yet to be achieved and greater knowledge of the main processes governing the hydration of these materials is key to move forward.

This project aims to combine molecular scale simulation with Kinetic Monte Carlo (KMC) methods to obtain the knowledge required to take a step further in the **design of ultra-reactive cements and pozzolans. On the one hand, molecular simulation provides very detailed information on processes which take place at atomic scale and energy barriers associated to each process. On the other hand, KMC simulations allow time savings in molecular simulations (nanoseconds) and studying chemical processes in macroscopic scales (minutes).**

As a result of the project, the cement and pozzolan hydration mechanism will be unveiled from molecular to microscopic scale, from nanoseconds to minutes, without pre-conceived assumptions or empirical data. Thanks to this, synthesis paths and additives, such as nanoseeds increasing material hydration rates, will be designed.

Scholarship description:

- **Research Lines**

The project will have three well differentiated phases aimed at studying hydration in materials of interest; i.e. main cement phases (alite and belite) and pozzolans (aluminosilicates). Nevertheless, the method is similar regardless of the material as it is based on atomistic simulations not

requiring any specific material input, but only knowledge of atomic interactions. The three phases can be summarised as follows:

a) Methodology development: One of the main molecular simulation challenges is to transfer acquired knowledge from nanometric scale to macroscale. Kinetic Monte Carlo (KMC) methods may fill this gap using inter-atomic processes information to simulate the behaviour of materials for minutes. A KMC code is created in the first phase to study relevant phenomena during material dissolution: transport and desorption of solid units.

b) Molecular scale: In this part of the sub-project, materials will be researched using *ab-initio* atomistic simulation and molecular dynamics simulation methods. Energy barriers associated to material dissolution processes will be determined and used as input in our KMC code.

c) Microscopic scale: with the information obtained at molecular scale and the KMC code developed, factors affecting hydration of cement and pozzolan phases will be studied. Among other factors we will research particle size impact, aspect/size ratios, crystal shapes, impurities, accelerator impact, etc.

- **Goals**

The ultimate aim is to determine cement and pozzolan hydration mechanism from molecular to microscopic scale and from nanoseconds to minutes and use the information obtained to propose new hydration accelerators (nanoseeds, chemical accelerators) or synthesis methods modifying cement phases to increase reactivity.

- **Projects for activity application**

GEI Green Concrete Design Project, EMAITEK (nanoseeds) and ETORTEK

- **PhD University and Doctoral Supervision Agreement**

  An agreement with Professor Iñigo López Arbeloa of the Chemistry Physics Department of the University of the Basque Country (UPV/EHU) Faculty of Science and Technology has been reached to host this PhD.

Requirements:

The PhD candidate shall meet the following requirements:

- Qualification and Speciality: Degree/Diploma in Physics, Science Computing speciality
- Languages: English (intermediate/advanced)
- IT skills: Programming in FORTRAN and C++, Matlab, UNIX languages

- The following will be a plus: Academic record grades; Masters degree related to the project.